

## **A New Method for Determination of the Intermolecular Potential Parameters**

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At present, computer simulation of fluids is carried out more and more. But first we must know the intermolecular potential parameters of fluids. In other words, it is essential for computer simulation to predict the behavior or thermodynamic properties or transport properties of fluids. Usually, the PVT properties, viscosity or Joule-Thomson coefficients are used for the determination of the intermolecular potential parameters. But we know that it is difficult to get high accuracy experiment data of those properties. Recently, much attention has been given to measurements of the sound speeds of fluids, and now we can get sound speed with very high accuracy (better than 0.01%). Thus, we want to determine the intermolecular potential parameters from the sound speed. In this paper, we have deduced some formulations of the second acoustical virial coefficient and intermolecular potential functions (including Lennard-Jones, Kihara, Stockmayer, etc.). With these formulations and nonlinear least squares method, we can obtain intermolecular potential parameters directly from the sound speeds of fluids. In order to test this method, we use it to determine the Lennard-Jones, Kihara, and Stockmayer potential parameters of the refrigerant HFC-125, and then we calculate the second virial coefficient with those potential functions and parameters. We found the calculated second virial coefficients agreed well with experimental data.